Soft X-ray Emission and Absorption Spectra of Oxygen Incorporated in Microporous Carbon

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Microporous carbon has been widely used for adsorbents and catalysts in many industrial fields. Its adsorption properties were thought likely to depend on the surface structure and chemical states of the graphitic surface in the micropores. One of the most important surface-structure/chemical-states is the oxidation state of the graphitic surface. The oxidized surface structure in microporous carbon has been estimated from thermally desorbed gaseous fractions by the gas-phase chemical modification method, which can be regarded as an *indirect* method of detecting oxygen. We therefore measured synchrotron-radiation-excited O *K* x-ray emission and absorption spectra of oxygen incorporated in microporous carbon using a grating x-ray spectrometer in BL-8.0.1, in order to *directly* observe the oxygen and identify its chemical states on the graphitic surface in microporous carbon [1, 2]. Figure 1 shows the soft x-ray emission and the fluorescence-yield (FY) x-ray absorption spectra of the commercially obtained microporous carbon in the O *K* region. The O *K* x-ray emission spectrum exhibited a peak at 526 eV with a low-energy tail, and the absorption spectrum at the O *K* threshold exhibited a sharp peak at 531.5 eV and then rose from 535 eV. Spectral feature analysis using DV-Xα molecular orbital calculations showed that the measured x-ray spectra were not sufficiently explained by the typical -OH substituent on the graphitic surface, nor by adsorbed H_2O. Further theoretical analysis, using more complicated cluster models having other substituents and backbone structures, of these x-ray spectra is in progress to determine the chemical states of oxygen on the graphitic surface in microporous carbon.

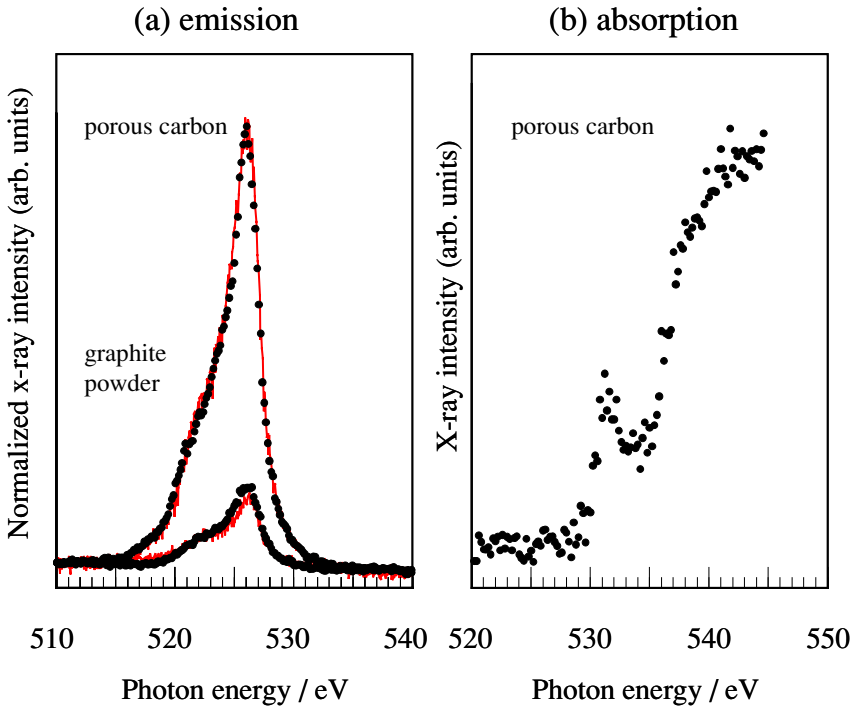

Figure 1. Soft x-ray emission spectra of microporous carbon and graphite powder (left panel) and FY x-ray absorption spectra of microporous carbon (right) in the O *K* region.

[1] Y. Muramatsu et al., Carbon (in press), [2] Y. Muramatsu et al., J. Electron Spectrosc. Relat. Phenom. (in press).

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